Self-Energy Correction to the Hyperfine Splitting for Excited States

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The self-energy corrections to the hyperfine splitting is evaluated for higher excited states in hydrogenlike ions, using an expansion in the binding parameter $Z\alpha$, where Z is the nuclear charge number, and α is the fine-structure constant. We present analytic results for D, F and G states, and for a number of highly excited Rydberg states with principal quantum numbers in the range $13 \leq n \leq 16$, and orbital angular momenta $\ell = n-2$ and $\ell = n-1$. A closed-form, analytic expression is derived for the contribution of high-energy photons, valid for any state with $\ell \geq 2$ and arbitrary n, ℓ and total angular momentum j. The low-energy contributions are written in the form of generalized Bethe logarithms and evaluated for selected states.

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I. INTRODUCTION

The self-energy correction to the hyperfine splitting is the dominant quantum electrodynamic (QED) correction to the magnetic interaction of the bound electron with the field of the nucleus. The hyperfine interaction energy of electron and nucleus is proportional to $g_N\,\alpha(Z\alpha)^3 m_e^2/m_N$, where g_N is the nuclear g factor, and m_e and m_N are the electron and nuclear masses, respectively. Relativistic corrections enter at relative order $(Z\alpha)^2$. The dominant QED correction is due to the anomalous magnetic moment of the electron and enters at relative order α. Here, we consider the QED correction of order $\alpha\,(Z\alpha)^2$, which is the sum of a high- and a low-energy part. Relativistic corrections to the anomalous magnetic interaction give one of the dominant contributions to the high-energy part, which can otherwise be calculated on the basis of a form-factor approach, using a generalized Dirac equation in which the radiative effects and the hyperfine interaction are inserted "by hand." The low-energy part constitutes a correction to the Bethe logarithm due to the hyperfine interaction. It can be formulated as a hyperfine correction to the self-energy, the effect being equivalent to the self-energy correction to the hyperfine splitting mediated by low-energy virtual photons [up to order $\alpha\,(Z\alpha)^2$].

In our treatment, we follow the formalism of nonrelativistic QED (NRQED) detailed in Ref. [1], and refer to Refs. [2–7] for a number of previous investigations regarding the treatment of the self-energy correction to the hyperfine splitting in systems with low nuclear charge number.

Our paper is organized as follows. The general formalism of the hyperfine interaction is described in Sec. II. For the self-energy correction, the low-energy part is treated in Sec. III, and the high-energy part is calculated in Sec. IV. Results and theoretical predictions are discussed in Sec. V. Conclusions are reserved for Sec. VI. Natural units with $\hbar = c = \epsilon_0 = 1$ are used throughout the paper.

II. FORMALISM

Following the derivation in Ref. [8], the magnetic dipole field of the nucleus is described by the vector potential

$$\vec{A}_{\rm hfs}(\vec{x}) = -\frac{1}{4\pi}\frac{\vec{\mu}\times\vec{x}}{r^3}\,, \tag{1}$$

where $\vec{x}$ is the coordinate vector and $r = |\vec{x}|$. The curl of this vector potential yields the magnetic field

$$\vec{B}_{\rm hfs} = \vec{\nabla}\times\vec{A}_{\rm hfs}(\vec{x}) = -\frac{2}{3}\,\vec{\mu}\,\delta(\vec{x}) - \frac{3(\vec{\mu}\cdot\hat{\vec{x}})\hat{\vec{x}} - \vec{\mu}}{4\pi r^3}\,, \tag{2}$$

and the fully relativistic hyperfine interaction Hamiltonian thus reads

$$H_{\rm hfs} = -e\vec{\alpha}\cdot\vec{A}_{\rm hfs}(\vec{x}) = \frac{e}{4\pi}\vec{\alpha}\cdot\frac{\vec{\mu}\times\vec{x}}{r^3} = \frac{e}{4\pi}\vec{\mu}\cdot\frac{\vec{x}\times\vec{\alpha}}{r^3} \tag{3}$$

The hyperfine interaction couples Dirac eigenstates to the magnetic field of the nucleus. The electronic states can be written as $|njm\rangle \equiv |nj\ell m\rangle$, where n is the principal quantum number, and the orbital and total angular momenta of the electron (ℓ and j, respectively) can be mapped to the Dirac angular quantum number $\kappa = (-1)^{j-\ell+\frac{1}{2}}(j+\frac{1}{2})$. Finally, m is the projection of the total electron angular momentum onto the quantization axis. In this article, we sometimes suppress the orbital angular momentum ℓ in the notation because we consider the coupling of the total electron angular momentum j to the nuclear spin. Nuclear states are denoted as $|IM\rangle$, where I is the nuclear spin and M its projection onto the quantization axis. They are coupled to the electron eigenstates $|njm\rangle$ by the hyperfine interaction, to form states with quantum number $|nfm_fIj\rangle$ which are eigenstates of the total Dirac+hyperfine Hamiltonian (f is the total electron+nuclear angular momentum, and m_f is its projection). Using Clebsch–Gordan coefficients $C^{fm_f}_{IMjm}$, the $|nfm_fIj\rangle$ states can be written as

$$|nfm_fIj\rangle = \sum_{M,m} C^{fm_f}_{IMjm}\,|IM\rangle\,|njm\rangle\;. \tag{4}$$

The hyperfine energy $\Delta E_{\rm hfs}$ thus reads

$$E_{\rm hfs} = \langle n f m_f I j \, | H_{\rm hfs} | \, n f m_f I j \rangle \, . \quad (5)$$

Using the Wigner–Eckhart theorem, the hyperfine energy can be rewritten as

$$E_{\rm hfs} = \alpha \frac{g_N}{2} \frac{m_e}{m_N} \left[f(f+1) - I(I+1) - j(j+1) \right] \times \left\langle n j \tfrac{1}{2} \left| \frac{[\vec{x}\times\vec{\alpha}]_0}{m_e r^3} \right| n j \tfrac{1}{2} \right\rangle , \quad (6)$$

where $|nj\frac{1}{2}\rangle$ is the Dirac eigenstate with a definite angular momentum projection $+\frac{1}{2}$, and $[\vec{x}\times\vec{\alpha}]_0$ is the z component (zero component in the spherical basis) of the indicated vector product.

We have thus separated the nuclear from the electronic variables. A detailed analysis of the separation of the nuclear variables can also be found in Ref. [2]. This procedure allows to reduce the evaluations of the hyperfine structure and corrections to it, to the evaluation of matrix elements of operators acting solely on electronic states. Specifically, we consider corrections to the state-dependent electronic matrix element Θ_e, where

$$\Theta_e = \left\langle n j \tfrac{1}{2} \left| \frac{[\vec{x}\times\vec{\alpha}]_0}{m_e r^3} \right| n j \tfrac{1}{2} \right\rangle . \quad (7)$$

The hyperfine interaction energy thus is

$$E_{\rm hfs} = \alpha \frac{g_N}{2} \frac{m_e}{m_N} \left[f(f+1) - I(I+1) - j(j+1) \right] \Theta_e \, . \quad (8)$$

Relativistic atomic theory leads to the following result for Θ_e (see Refs. [4, 9])

$$\Theta_e = (Z\alpha)^3 m_e \frac{\kappa(2\kappa(\gamma + n - |\kappa|) - N)}{N^4 \left(\kappa^2 - \frac{1}{4}\right) \gamma (4\gamma^2 - 1)} , \quad (9)$$

where $\gamma = \sqrt{\kappa^2 - (Z\alpha)^2}$. The effective principal quantum number is $N = \sqrt{(n-|\kappa|)^2 + 2(n-|\kappa|)\gamma + \kappa^2}$.

III. LOW-ENERGY PART

A. General Formalism

In order to treat low-energy virtual photons, we apply a Foldy-Wouthuysen transformation to the total Hamiltonian H_t which is the sum of the Dirac–Coulomb Hamiltonian and the relativistic hyperfine interaction Hamiltonian,

$$H_t = H_D + H_{\rm hfs} = \vec{\alpha}\cdot\vec{p} + \beta m_e - \frac{Z\alpha}{r} - e\,\vec{\alpha}\cdot\vec{A}_{\rm hfs}(\vec{x}) \, . \quad (10)$$

The Foldy-Wouthuysen transformation of this Hamiltonian is carried out as described in Refs. [7, 8, 10–12]. The only difference to the case of the ordinary Dirac Hamiltonian is that the odd operator $\mathcal{O}$ used in the construction of the transformation [11] now reads

$$\mathcal{O} = \vec{\alpha}\cdot\vec{p} - e\,\vec{\alpha}\cdot\vec{A}_{\rm hfs}(\vec{x}) \quad (11)$$

instead of $\vec{\alpha}\cdot\vec{p}$. The result of the transformation,

$$H_t' + U H_t U^{-1} = H_{\rm FW} + H_{\rm HFS} \, , \quad (12)$$

is the sum of the Foldy-Wouthuysen Hamiltonian $H_{\rm FW}$ from Ref. [10], and $H_{\rm HFS}$ is the nonrelativistic hyperfine splitting Hamiltonian [2, 8]

$$H_{\rm HFS} = \frac{e\,m_e}{4\pi} \vec{\mu}\cdot\vec{h} = \frac{e\,m_e}{4\pi} \vec{\mu}\cdot\left(\vec{h}_S + \vec{h}_D + \vec{h}_L\right) . \quad (13)$$

It consists of the three parts,

$$\vec{h}_S = \frac{4\pi}{3m_e^2} \vec{\sigma}\,\delta(\vec{x}) \, , \quad (14a)$$

$$\vec{h}_D = \frac{3(\vec{\sigma}\cdot\hat{x})\hat{x} - \vec{\sigma}}{2m_e^2 r^3} \, , \quad (14b)$$

$$\vec{h}_L = \frac{\vec{\ell}}{m_e^2 r^3} \, , \quad (14c)$$

whose designation is inspired by the apparent angular momentum association of the terms. Following the notation in Ref. [8], lowercase letters in the subscript are used to label relativistic operators, whereas nonrelativistic operators are denoted by uppercase letters in the subscript. However, we use the lowercase notation for the scaled vector quantity $\vec{h}$ in order to denote the electronic operators in the nonrelativistic hyperfine Hamiltonian. Furthermore, $\hat{x} = \vec{x}/|\vec{x}|$ is the position unit vector. The zero component (z component) $h_0 = h_{S,0} + h_{D,0} + h_{L,0}$ of the Hamiltonian "vector" $\vec{h}$ therefore reads as

$$h_0 = \frac{4\pi}{3m_e^2} \sigma_0\,\delta(\vec{x}) + \frac{3(\vec{\sigma}\cdot\hat{x})\hat{x}_0 - \sigma_0}{2m_e^2 r^3} + \frac{\ell_0}{m_e^2 r^3} \, . \quad (15)$$

With the help of h_0, the nonrelativistic limit of Eq. (9) is obtained as

$$\Theta_e^{\rm NR} = \langle n j \ell \tfrac{1}{2} \, | h_0 | \, n j \ell \tfrac{1}{2} \rangle = \frac{\kappa}{|\kappa|} \, \frac{(Z\alpha)^3 m_e}{n^3 (2\kappa + 1)(\kappa^2 - \frac{1}{4})} , \quad (16)$$

which we use to define the nonrelativistic quantity

$$E_F = E_{\rm HFS}^{\rm NR} = E_{\rm HFS} = \alpha \frac{g_N}{2} \frac{m_e}{m_N} \times \left[f(f+1) - I(I+1) - j(j+1) \right] \Theta_e^{\rm NR} , \quad (17)$$

which is commonly referred to as the Fermi energy. The relativistic and QED corrections can be expressed as multiplicative corrections of Θ_e, via the replacement

$$\Theta_e^{\rm NR} \to \Theta_e^{\rm NR} \left[1 + \delta\Theta_e^{\rm rel} + \delta\Theta_e^{\rm QED} \right] . \quad (18)$$

By expanding Θ_e to second order in $Z\alpha$, we obtain

$$\delta\Theta_e^{\rm rel} = (Z\alpha)^2 \left(\frac{12\kappa^2-1}{2\kappa^2(2\kappa-1)(2\kappa+1)} + \frac{3}{2n}\frac{1}{|\kappa|} + \frac{3-8\kappa}{2n^2(2\kappa-1)} \right) \tag{19}$$

and the corresponding energy shift

$$\delta E_{\rm hfs}^{\rm rel} = E_{\rm HFS}\, \delta\Theta_e^{\rm rel} \,. \tag{20}$$

The QED term

$$\delta E_{\rm HFS}^{\rm QED} = E_{\rm HFS}\, \delta\Theta_e^{\rm QED} \tag{21}$$

is the subject of this paper. For the QED corrections terms up to relative order $\alpha(Z\alpha)^2$ with respect to the nonrelativistic hyperfine splitting will be considered. In order to do the calculation, we need the three terms from Eq. (13) and a further correction to the electron's transition current, due to the hyperfine interaction. Namely, in the presence of the hyperfine interaction, the kinetic momentum of the electron finds a modification

$$\frac{\vec p}{m_e} \to \frac{\vec p}{m_e} - \frac{e}{m_e}\vec A_{\rm hfs} = \frac{\vec p}{m_e} + \frac{|e|\, m_e}{4\pi}\, |\vec\mu|\, \delta\vec\jmath_{\rm HFS} \,. \tag{22}$$

The current

$$\delta\vec\jmath_{\rm HFS} = \frac{\hat{\vec\mu} \times \vec x}{m_e^2 r^3} \tag{23}$$

has the zero component

$$\delta\vec\jmath_{0,\rm HFS} = \frac{1}{m_e^2 r^3}\left(-y\,\hat e_x + x\,\hat e_y\right) , \tag{24}$$

which is used in the calculations below.

B. Specific Terms

Following Ref. [8], there are four corrections, which arise from the correction of the interaction current, from the correction of the Hamiltonian, from the correction of the reference state energy, and finally from the correction of the reference-state wave function. We first treat the hyperfine correction to the interaction current and to this end, define a useful normalization factor

$$\mathcal{N} = \frac{1}{\langle nj\ell\tfrac12\, |h_0|\, nj\ell\tfrac12\rangle} = \frac{1}{\Theta_e^{\rm NR}} \,. \tag{25}$$

The hyperfine correction to the interaction current is then given as

$$\begin{aligned}
\delta\Theta_L^{\delta j} &= \frac{4\alpha\mathcal{N}}{3\pi} \int_0^\epsilon {\rm d}\omega_{\vec k}\omega_{\vec k} \sum_{n'j'\ell'm'} \left\langle nj\ell\tfrac12 \left| \frac{p^i}{m_e} \right| n'j'\ell'm' \right\rangle \\
&\times \frac{1}{E_n - E_{n'} - \omega_{\vec k}} \left\langle n'j'\ell'm' \left| \delta j^i_{0,\rm HFS} \right| nj\ell\tfrac12 \right\rangle \\
&= \frac{\alpha}{\pi}(Z\alpha)^2 \frac{4\mathcal{N}}{3(Z\alpha)^2} \sum_{n'j'\ell'm'} (E_n - E_{n'}) \ln\left(\frac{|E_{n'} - E_n|}{m_e (Z\alpha)^2} \right) \\
&\times \left\langle nj\ell\tfrac12 \left| \frac{p^i}{m_e} \right| n'j'\ell'm' \right\rangle \left\langle n'j'\ell'm' \left| \delta j^i_{0,\rm HFS} \right| nj\ell\tfrac12 \right\rangle .
\end{aligned} \tag{26}$$

The term containing the logarithm of ϵ, which is a scale-separation parameter that cancels when high- and low-energy parts are added [13], vanishes after angular integration in the matrix element. The structure of the logarithmic term here is very similar to the Bethe logarithm encountered in Ref. [14]. Terms of this form will arise for the other corrections in the low-energy part as well. In the following, these terms are denoted as $\beta_{\rm HFS}$ and are evaluated numerically with the methods described in Ref. [15]. Thus, the low-energy correction due to the nuclear-spin dependent current is

$$\delta\Theta_L^{\delta j} = \frac{\alpha}{\pi}(Z\alpha)^2 \beta_{\rm HFS}^{\delta j} \,. \tag{27}$$

Next, we treat the corrections to the Hamiltonian, to the energy and to the wave function. The perturbation due to the hyperfine splitting Hamiltonian yields the term [we define the resolvent $G(\omega_{\vec k}) = 1/(E_n - H_S - \omega_{\vec k})$]

$$\begin{aligned}
\delta\Theta_L^{\delta H} &= \frac{2\alpha\mathcal{N}}{3\pi} \int_0^\epsilon {\rm d}\omega_{\vec k}\, \omega_{\vec k} \\
&\times \left\langle nj\ell\tfrac12 \left| \frac{p^i}{m_e} G(\omega_{\vec k})\, h_0\, G(\omega_{\vec k}) \frac{p^i}{m_e} \right| nj\ell\tfrac12 \right\rangle \\
&= \frac{2\alpha\mathcal{N}}{3\pi m_e^2} \ln\left[\frac{\epsilon}{m_e (Z\alpha)^2} \right] \\
&\times \left\langle nj\ell\tfrac12 \left| \left(\frac12 [p^i, [h_0, p^i]] + p^2 h_0 \right) \right| nj\ell\tfrac12 \right\rangle \\
&\quad + \frac{\alpha}{\pi}(Z\alpha)^2 \beta_{\rm HFS}^{\delta H} ,
\end{aligned} \tag{28}$$

The correction to the energy denominator in the

Schrödinger propagator can be written as

$$\begin{aligned}\delta\Theta_L^{\delta E} &= -\frac{2\alpha\mathcal{N}}{3\pi}\int_0^\epsilon d\omega_{\vec{k}}\,\omega_{\vec{k}}\,\langle nj\ell\tfrac{1}{2}\,|h_0|\,nj\ell\tfrac{1}{2}\rangle\\ &\quad\times\left\langle nj\ell\tfrac{1}{2}\left|\frac{p^i}{m_e}\left[G(\omega_{\vec{k}})\right]^2\frac{p^i}{m_e}\right|nj\ell\tfrac{1}{2}\right\rangle\\ &= -\frac{2\alpha\mathcal{N}}{3\pi m_e^2}\ln\left[\frac{\epsilon}{m_e(Z\alpha)^2}\right]\langle nj\ell\tfrac{1}{2}\,|p^2|\,nj\ell\tfrac{1}{2}\rangle\\ &\quad\times\langle nj\ell\tfrac{1}{2}\,|h_0|\,nj\ell\tfrac{1}{2}\rangle+\frac{\alpha}{\pi}(Z\alpha)^2\beta_{\rm HFS}^{\delta E}\,,\end{aligned}\tag{29}$$

where the prime indicates the reduced Green function. Finally, the correction to the wave function due to the hyperfine splitting Hamiltonian is

$$\begin{aligned}\delta\Theta_L^{\delta\Phi} &= \frac{4\alpha\mathcal{N}}{3\pi}\int_0^\epsilon d\omega_{\vec{k}}\,\omega_{\vec{k}}\\ &\times\left\langle nj\ell\tfrac{1}{2}\left|\frac{p^i}{m_e}G(\omega_{\vec{k}})\frac{p^i}{m_e}\left(\frac{1}{E_n-H_S}\right)'h_0\right|nj\ell\tfrac{1}{2}\right\rangle\\ &= \frac{4\alpha\mathcal{N}}{3\pi m_e^2}\ln\!\left[\frac{\epsilon}{m_e(Z\alpha)^2}\right]\\ &\quad\times\left\langle nj\ell\tfrac{1}{2}\left|p^i(H_S-E_n)p^i\left(\frac{1}{E_n-H_S}\right)'h_0\right|nj\ell\tfrac{1}{2}\right\rangle\\ &\qquad+\frac{\alpha}{\pi}(Z\alpha)^2\beta_{\rm HFS}^{\delta\Phi}\,.\end{aligned}\tag{30}$$

Using commutator relations, one can finally sum up all four corrections in the low-energy part to

$$\begin{aligned}\delta\Theta_L &= \delta\Theta_L^{\delta j}+\delta\Theta_L^{\delta H}+\delta\Theta_L^{\delta E}+\delta\Theta_L^{\delta\Phi}\\ &= \frac{\alpha\mathcal{N}}{3\pi m_e^2}\ln\left[\frac{\epsilon}{m_e(Z\alpha)^2}\right]\langle nj\ell\tfrac{1}{2}\,|[p^i,[h_0,p^i]]|\,nj\ell\tfrac{1}{2}\rangle\\ &\quad+\frac{\alpha}{\pi}(Z\alpha)^2\beta_{\rm HFS}\,,\end{aligned}\tag{31}$$

where $\beta_{\rm HFS}$ is the sum

$$\beta_{\rm HFS}=\beta_{\rm HFS}^{\delta j}+\beta_{\rm HFS}^{\delta H}+\beta_{\rm HFS}^{\delta E}+\beta_{\rm HFS}^{\delta\Phi}\,.\tag{32}$$

The double commutator

$$\langle nj\ell\tfrac{1}{2}\,|[p^i,[h_0,p^i]]|\,nj\ell\tfrac{1}{2}\rangle=\left\langle nj\ell\tfrac{1}{2}\left|\vec{\nabla}^2h_0\right|nj\ell\tfrac{1}{2}\right\rangle\tag{33}$$

vanishes for states with $\ell\geq 2$ up to and including order $(Z\alpha)^5$, and hence $\delta\Theta_L$ takes the very simple form

$$\delta\Theta_L=\frac{\alpha}{\pi}(Z\alpha)^2\beta_{\rm HFS}\,.\tag{34}$$

IV. HIGH-ENERGY PART

Up to relative order $\alpha(Z\alpha)^2E_F$, it is sufficient [8] to consider the problem on the level of the modified Dirac Hamiltonian

$$\begin{aligned}H_D^{(m)} &= \vec{\alpha}\left[\vec{p}-eF_1(\vec{\nabla}^2)\vec{A}\right]+\beta m_e+F_1(\vec{\nabla}^2)V\\ &\quad+F_2(\vec{\nabla}^2)\frac{e}{2m_e}\left(\mathrm{i}\vec{\gamma}\cdot\vec{E}-\beta\,\vec{\Sigma}\cdot\vec{B}\right)\,,\end{aligned}\tag{35}$$

where F_1 and F_2 are the one-loop Dirac and Pauli form factors of the electron, respectively. Their expressions are known (see Chapter 7 of Ref. [16]).

The F_1 form factor slope gives rise to the following effective interaction

$$-eF_1'(0)\vec{\nabla}^2\vec{\alpha}\cdot\vec{A}_{\rm hfs}=\frac{\alpha}{3\pi}\left[\ln\left(\frac{m_e}{2\epsilon}\right)+\frac{11}{24}\right]\vec{\nabla}^2H_{\rm hfs}\,.\tag{36}$$

Up to the order $\alpha(Z\alpha)^2E_F$, we may write the correction in terms of the nonrelativistic hyperfine Hamiltonian h_0,

$$\delta\Theta_{H,1}=\frac{\alpha\mathcal{N}}{3\pi m_e^2}\left[\ln\left(\frac{m_e}{2\epsilon}\right)+\frac{11}{24}\right]\left\langle nj\ell\tfrac{1}{2}\left|\vec{\nabla}^2h_0\right|nj\ell\tfrac{1}{2}\right\rangle\,.\tag{37}$$

However, as already pointed out, the matrix element of $\vec{\nabla}^2h_0$ vanishes on states with $\ell\geq 2$ which are relevant to our investigations, and so

$$\delta\Theta_{H,1}=0\,.\tag{38}$$

The second correction is a second-order perturbation involving the F_1 correction to the Coulomb potential,

$$\begin{aligned}\delta\Theta_{H,2} &= \frac{2\alpha\mathcal{N}}{3\pi m_e^2}\left[\ln\left(\frac{m_e}{2\epsilon}\right)+\frac{11}{24}\right]\\ &\quad\times\left\langle nj\ell\tfrac{1}{2}\left|\vec{\nabla}^2V\left(\frac{1}{E_n-H_S}\right)'h_0\right|nj\ell\tfrac{1}{2}\right\rangle\,.\end{aligned}\tag{39}$$

Again, $\vec{\nabla}^2V$ is proportional to the Dirac δ and therefore vanishes for states with $\ell\geq 1$. Accordingly, for states with $\ell\geq 2$ we have

$$\delta\Theta_{H,2}=0\,.\tag{40}$$

The Pauli F_2 form factor gives rise to a second-order perturbation involving a magnetic moment correction to the Coulomb potential,

$$\begin{aligned}\delta\Theta_{H,3} &= 2\mathcal{N}\,F_2(0)\\ &\quad\times\left\langle\psi^\dagger\left|\frac{-\mathrm{i}}{2m_e}\vec{\gamma}\cdot\vec{\nabla}V\left(\frac{1}{E_\psi-H_D}\right)'H_{\rm hfs}\right|\psi\right\rangle\,,\end{aligned}\tag{41}$$

where F_2 is the magnetic form factor. For $F_2(0)$, the Schwinger value $F_2(0)=\frac{\alpha}{2\pi}$ may be used. After a Foldy–Wouthuysen transformation, we can write $\delta\Theta_{H,3}$ as the sum of two terms. The first of these, $\delta\Theta_{H,3n}$, involves no mixing of upper and lower components in the Dirac wave function and reads

$$\begin{aligned}\delta\Theta_{H,3n} &= \frac{\alpha\mathcal{N}}{2\pi m_e^2}\\ &\times\left\langle nj\ell\tfrac{1}{2}\left|\frac{Z\alpha}{r^3}\vec{\sigma}\cdot\vec{\ell}\left(\frac{1}{E_n-H_S}\right)'H_{\rm HFS}\right|nj\ell\tfrac{1}{2}\right\rangle\,.\end{aligned}\tag{42}$$

We find the following general result for states with $\ell \geq 2$,

$$\delta\Theta_{H,3n} = \frac{\alpha}{\pi}(Z\alpha)^2 \left(\frac{1}{2\ell\kappa} \, \frac{60\ell^4 + 120\ell^3 + 55\ell^2 - 5\ell - 3}{(2\ell+1)^2\,(4\ell^3 + 8\ell^2 + \ell - 3)} + \frac{3}{2n}\,\frac{1}{\kappa(2\ell+1)} - \frac{3}{8n^2}\,\frac{\ell(\ell+1)}{\kappa(\ell+\frac{3}{2})(\ell-\frac{1}{2})} \right) . \quad (43)$$

Lower components of the Dirac wave function give rise to the mixing term

$$\begin{aligned}\delta\Theta_{H,3m} &= -\,\mathrm{i}\frac{\alpha\mathcal{N}}{2\pi m_e} \left\langle nj\ell\tfrac{1}{2} \left| \frac{Z\alpha}{r^3}\,(\vec{\gamma}\cdot\vec{x})\,\frac{1}{2m_e} H_{\rm hfs} \right| nj\ell\tfrac{1}{2} \right\rangle \\ &= \frac{\alpha\mathcal{N}}{\pi}\,\frac{-\kappa}{8j(j+1)} \left\langle nj\ell\tfrac{1}{2} \left| \frac{Z\alpha}{m_e^3 r^4} \right| nj\ell\tfrac{1}{2} \right\rangle . \quad (44)\end{aligned}$$

We find the general result

$$\delta\Theta_{H,3m} = \frac{\alpha}{\pi}(Z\alpha)^2 \frac{|\kappa|}{4j(j+1)}\,\frac{(2\kappa+1)(\kappa^2-\frac{1}{4})}{(2\ell-1)(2\ell+3)(\ell+\frac{1}{2})} \times \left(\frac{1}{n^2} - \frac{3}{\ell(\ell+1)} \right) . \quad (45)$$

The F_2 correction to the magnetic photon exchange of electron and nucleus gives rise to the effective interaction

$$-F_2(\vec{\nabla}^2)\frac{e}{2m_e}\beta\,\vec{\Sigma}\cdot\vec{B}_{\rm hfs} = F_2(\vec{\nabla}^2)\left[\frac{em_e}{4\pi}\beta\vec{\mu}\cdot\left(\vec{h}_s + \vec{h}_d\right)\right] . \quad (46)$$

Here, $\vec{h}_s$ and $\vec{h}_d$ are the generalizations of $\vec{h}_S$ and $\vec{h}_D$ to 4×4 matrices,

$$\vec{h}_s = \frac{4\pi}{3m_e^2}\,\vec{\Sigma}\,\delta(\vec{x})\,, \quad (47a)$$

$$\vec{h}_d = \frac{3\,(\vec{\Sigma}\cdot\hat{\vec{x}})\,\hat{\vec{x}} - \vec{\Sigma}}{2\,m_e^2\,r^3} . \quad (47b)$$

Taking $F_2(\vec{\nabla}^2) \approx F_2(0)$ in Eq. (46), we obtain the correction

$$\begin{aligned}\delta\Theta_{H,4} &= \mathcal{N} F_2(0)\,\langle\psi\,|\beta\,(h_{s,0} + h_{d,0})|\,\psi\rangle \\ &= \frac{\alpha\mathcal{N}}{2\pi}\,\langle\psi\,|\beta\,(h_{s,0} + h_{d,0})|\,\psi\rangle . \quad (48)\end{aligned}$$

Generalizing results from Ref. [17] for the term of relative order α, we find the result

$$\delta\Theta_{H,4} = \frac{\alpha}{\pi}\left[\frac{1}{4\kappa} + (Z\alpha)^2\left(\frac{24\kappa^3 + 18\kappa^2 - \kappa - 1}{8\kappa^3(4\kappa^3 + 4\kappa^2 - \kappa - 1)} + \frac{3}{8n}\,\frac{1}{|\kappa|\kappa} + \frac{1}{n^2}\,\frac{1}{2\kappa}\,\frac{1-3\kappa}{2\kappa-1}\right)\right] . \quad (49)$$

Taking the slope of F_2 in Eq. (46), we obtain

$$\begin{aligned}&F_2'(0)\frac{e}{2m_e}\beta\,\vec{\nabla}^2\,\vec{\Sigma}\cdot\vec{B}_{\rm hfs} \\ &\quad = \frac{\alpha}{12\pi}\left[\frac{em_e}{4\pi}\beta\vec{\mu}\cdot\left\{\vec{\nabla}^2\left(\vec{h}_s + \vec{h}_d\right)\right\}\right] , \quad (50)\end{aligned}$$

TABLE I: Low-energy contribution $\beta_{\rm HFS}$ of the self-energy correction for the hyperfine splitting for D states ($\ell = 2$).

n	$\beta_{\rm HFS}(nD_{3/2})$	$\beta_{\rm HFS}(nD_{5/2})$
3	$-2.068\ 39(5) \times 10^{-2}$	$-3.455\ 22(5) \times 10^{-2}$
4	$-1.302\ 99(5) \times 10^{-2}$	$-3.793\ 94(5) \times 10^{-2}$
5	$-1.025\ 92(5) \times 10^{-2}$	$-3.965\ 95(5) \times 10^{-2}$
6	$-0.943\ 28(5) \times 10^{-2}$	$-4.084\ 82(5) \times 10^{-2}$

TABLE II: Low-energy contribution $\beta_{\rm HFS}$ of the self-energy correction for the hyperfine splitting for F states ($\ell = 3$).

n	$\beta_{\rm HFS}(nF_{5/2})$	$\beta_{\rm HFS}(nF_{7/2})$
4	$-1.021\ 46(5) \times 10^{-2}$	$-0.953\ 04(5) \times 10^{-2}$
5	$-0.683\ 94(5) \times 10^{-2}$	$-1.077\ 62(5) \times 10^{-2}$
6	$-0.504\ 64(5) \times 10^{-2}$	$-1.141\ 28(5) \times 10^{-2}$
7	$-0.407\ 32(5) \times 10^{-2}$	$-1.182\ 43(5) \times 10^{-2}$

TABLE III: Low-energy contribution $\beta_{\rm HFS}$ of the self-energy correction for the hyperfine splitting for G states ($\ell = 4$).

n	$\beta_{\rm HFS}(nG_{7/2})$	$\beta_{\rm HFS}(nG_{9/2})$
5	$-0.368\ 23(5) \times 10^{-2}$	$-0.341\ 76(5) \times 10^{-2}$
6	$-0.147\ 39(5) \times 10^{-2}$	$-0.388\ 58(5) \times 10^{-2}$
7	$-0.012\ 93(5) \times 10^{-2}$	$-0.414\ 24(5) \times 10^{-2}$
8	$0.072\ 16(5) \times 10^{-2}$	$-0.430\ 98(5) \times 10^{-2}$

with $F_2'(0) = \alpha/12\pi$. As $F_2'(0)\vec{\nabla}^2$ already is of relative order $\alpha(Z\alpha)^2$, this operator only has to be applied to the nonrelativistic wave function where it vanishes for states with $\ell \geq 2$ and thus

$$\delta\Theta_{H,5} = \frac{\alpha\mathcal{N}}{12\pi}\left\langle nj\ell\tfrac{1}{2}\left|\vec{\nabla}^2\,(h_{S,0} + h_{D,0})\right| nj\ell\tfrac{1}{2}\right\rangle = 0 . \quad (51)$$

Finally, since

$$\delta\Theta_{H,1} = \delta\Theta_{H,2} = \delta\Theta_{H,5} = 0\,, \quad (52)$$

we have for the high-energy part the result

$$\delta\Theta_H = \delta\Theta_{H,3n} + \delta\Theta_{H,3m} + \delta\Theta_{H,4} . \quad (53)$$

It is quite surprising that the result obtained by adding

TABLE IV: Low-energy contribution $\beta_{\rm HFS}$ of the self-energy correction for the hyperfine splitting for highly excited states. The numbers in parentheses are standard uncertainties in the last figure. The exponent of the numerical data is chosen to be the same as in Tables I, II, and III, illustrating the monotonic decrease of the coeffcients with the angular momentum quantum numbers.

n	ℓ	$2j$	κ	$\beta_{\rm HFS}$	$2j$	κ	$\beta_{\rm HFS}$
16	15	29	15	$0.006\,310(5) \times 10^{-2}$	31	-16	$-0.002\,130(5) \times 10^{-2}$
16	14	27	14	$0.016\,397(5) \times 10^{-2}$	29	-15	$-0.003\,041(5) \times 10^{-2}$
15	14	27	14	$0.006\,888(5) \times 10^{-2}$	29	-15	$-0.002\,795(5) \times 10^{-2}$
15	13	25	13	$0.019\,372(5) \times 10^{-2}$	27	-14	$-0.004\,086(5) \times 10^{-2}$
14	13	25	13	$0.007\,420(5) \times 10^{-2}$	27	-14	$-0.003\,741(5) \times 10^{-2}$
14	12	23	12	$0.023\,029(5) \times 10^{-2}$	25	-13	$-0.005\,617(5) \times 10^{-2}$
13	12	23	12	$0.007\,794(5) \times 10^{-2}$	25	-13	$-0.005\,122(5) \times 10^{-2}$

the above expressions,

$$\begin{aligned}\delta\Theta_H = {} & \frac{\alpha}{\pi}\left\{\frac{1}{4\kappa} + (Z\alpha)^2\left[\frac{1}{8\kappa^3}\,\frac{24\kappa^3+18\kappa^2-\kappa-1}{4\kappa^3+4\kappa^2-\kappa-1}\right.\right.\\ & + \frac{1}{2\ell\kappa}\,\frac{60\ell^4+120\ell^3+55\ell^2-5\ell-3}{(2\ell+1)^2\,(4\ell^3+8\ell^2+\ell-3)}\\ & - \frac{3}{\ell(\ell+1)}\frac{j+\frac{1}{2}}{4j(j+1)}\frac{(2\kappa+1)(\kappa^2-\frac{1}{4})}{(2\ell-1)(2\ell+3)(\ell+\frac{1}{2})}\\ & + \frac{1}{n}\,\frac{3}{8\kappa}\,\frac{4(j+\frac{1}{2})+(2\ell+1)}{(2\ell+1)(j+\frac{1}{2})} + \frac{1}{8n^2}\left(\frac{4}{1-2\kappa}-\frac{4}{\kappa}\right.\\ & \left.\left.\left. + \frac{(2j+1)(2\kappa-1)(2\kappa+1)^2}{2j(j+1)(2\ell+3)\,(4\ell^2-1)} - \frac{3\ell(\ell+1)}{\kappa(\ell+\frac{3}{2})(\ell-\frac{1}{2})}\right)\right]\right\}.\end{aligned} \tag{54}$$

can actually be simplified quite considerably,

$$\begin{aligned}\delta\Theta_H = {} & \frac{\alpha}{\pi}\left\{\frac{1}{4\kappa} + (Z\alpha)^2\left[\frac{1}{n}\,\frac{3}{8}\,\frac{\kappa}{|\kappa|}\,\frac{6\kappa+1}{\kappa^2(2\kappa+1)}\right.\right.\\ & \left.\left. + \frac{1}{n^2}\,\frac{4\kappa-1}{2\kappa(1-2\kappa)} + \frac{(4\kappa+1)(6\kappa+1)(6\kappa^2+3\kappa-1)}{8\kappa^3(2\kappa+1)^2(2\kappa-1)(\kappa+1)}\right]\right\}.\end{aligned} \tag{55}$$

V. RESULTS AND PREDICTIONS

The total self-energy correction to the hyperfine splitting is obtained as the sum of the high- and low-energy parts given in Eqs. (55) and (34), which reads

$$\begin{aligned}\delta\Theta = {} & \frac{\alpha}{\pi}\left\{\frac{1}{4\kappa}\right.\\ & + (Z\alpha)^2\left[\frac{1}{8\kappa^3}\,\frac{(4\kappa+1)(6\kappa+1)(6\kappa^2+3\kappa-1)}{(2\kappa+1)^2(2\kappa-1)(\kappa+1)}\right.\\ & \left.\left. + \frac{1}{n}\,\frac{3}{8}\,\frac{\kappa}{|\kappa|}\,\frac{6\kappa+1}{\kappa^2(2\kappa+1)} + \frac{1}{n^2}\,\frac{4\kappa-1}{2\kappa(1-2\kappa)} + \beta_{\rm HFS}\right]\right\}.\end{aligned} \tag{56}$$

The Bethe logaritm type correction $\beta_{\rm HFS}$ is given in Eq. (32).

Restoring the reduced-mass dependence [we define $r(\mathcal{N}) \equiv m_e/m_N$] and adding the relativistic correction of relative order $(Z\alpha)^2$, we find that

$$\begin{aligned}\nu_{\rm hfs} = {} & R_\infty c\frac{Z^3\alpha^2}{n^3}\,\frac{r(\mathcal{N})}{[1+r(\mathcal{N})]^3}\,\frac{\kappa}{|\kappa|}\,\frac{g_N}{(2\kappa+1)(\kappa^2-\frac{1}{4})}\\ & \times [f(f+1)-I(I+1)-j(j+1)] \times \left\{1+(Z\alpha)^2\right.\\ & \times\left[\frac{12\kappa^2-1}{2\kappa^2(2\kappa-1)(2\kappa+1)} + \frac{3}{2n}\frac{1}{|\kappa|} + \frac{3-8\kappa}{2n^2(2\kappa-1)}\right]\\ & + \frac{\alpha}{\pi}\,\frac{1}{4\kappa} + \frac{\alpha}{\pi}(Z\alpha)^2\left[\frac{3}{8n}\,\frac{\kappa}{|\kappa|}\,\frac{6\kappa+1}{\kappa^2(2\kappa+1)} + \frac{1}{n^2}\,\frac{4\kappa-1}{2\kappa(1-2\kappa)}\right.\\ & \left.\left. + \frac{1}{8\kappa^3}\,\frac{(4\kappa+1)(6\kappa+1)(6\kappa^2+3\kappa-1)}{(2\kappa+1)^2(2\kappa-1)(\kappa+1)} + \beta_{\rm HFS}\right]\right\}.\end{aligned} \tag{57}$$

Numerical data for $\beta_{\rm HFS}$ for D, F, and G states, and selected Rydberg states, can be found in Tables I, II, III, and Table IV, respectively. The latter are relevant for a possible determination of fundamental constants from Rydberg state spectroscopy in hydrogenlike ions of medium nuclear charge number (see Ref. [18]).

A numerical example: For the transition $|1\rangle \leftrightarrow |2\rangle$ in atomic hydrogen ($Z = 1$) where

$$|1\rangle = |n=15, \ell=14, j=29/2, f=15\rangle\,, \tag{58}$$

$$|2\rangle = |n=16, \ell=15, j=31/2, f=16\rangle\,, \tag{59}$$

we find the following frequency shift from the Dirac value indicated in Eq. (2) of Ref. [17],

$$\Delta\nu_{{\rm hfs},1\to 2} = 96.759\,8630(8)\,{\rm Hz} + 78.764\,693(13)\,{\rm Hz}\,, \tag{60}$$

where the first term is due to the hyperfine effects calculated here, and the second term is due to relativistic recoil and QED effects calculated in Ref. [18]. The final theoretical prediction for the shift from the Dirac value

is

$$\Delta\nu_{\mathrm{hfs},1\to 2} = 175.524\,556(13)\,\mathrm{Hz}\,, \tag{61}$$

where the fundamental constants of CODATA 2006 [19] have been used in the numerical evaluation. The next higher-order term neglected here is the recoil correction of relative order $(Z\alpha)^2\, r(\mathcal{N})$, for which a general expression has been derived in Ref. [20] [the corresponding expression also is given in Eq. (42) of Ref. [4]]. The recoil correction is numerically suppressed for $Z = 1$.

VI. CONCLUSIONS

Rydberg states of hydrogenlike ions with medium nuclear charge number have been proposed as a device for the determination of fundamental constants [18]. Here, we demonstrate that it is possible to obtain accurate theoretical predictions for transition frequencies even in cases where the nucleus carries spin. To this end, we calculate the self-energy correction to the hyperfine splitting of the high-lying states. Vacuum polarization effects can be neglected for states with $\ell \geq 2$ to the order relevant for the current investigation.

We split the calculation into a low-energy part, which contains Bethe logarithm type corrections (Sec. III), and a high-energy part, which can be treated on the basis of electron form factors (Sec. IV). For the low-energy part, we find that the net result can be expressed as the sum of corrections due to the hyperfine Hamiltonian, due to the energy correction, due to the wave function correction, and due to the hyperfine modification of the electron's transition current. For the high-energy part, we find a sum of two terms, one of which is due to a second-order effect involving the Pauli form factor correction to the Coulomb field, and the second of which is an anomalous magnetic moment correction to the hyperfine splitting, evaluated on relativistic wave functions. The first correction can be split into two terms, which involve/do not involve mixing of the upper and lower components of the Dirac wave function, respectively. Quite surprisingly, the high-energy contribution can be expressed in closed analytic form, valid for an arbitrary excited state [see Eq. (55)]. For the Bethe logarithm type corrections relevant to the low-energy part, a numerical approach is indispensable.

Finally, as indicated in Tables I—III, we also find results for D, F, and G states which are of general interest to high-precision spectroscopy.

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